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First-principles modeling of energetic materials MIKE CONROY, University of South Florida, IVAN OLEYNIK, University of South Florida, CARTER WHITE, Naval Research Laboratory — The prediction of properties of energetic materials using atomic-scale simulation techniques is one of the promising areas of energetic materials (EM) research. One of the challenges is to understand the initial response of EM to shock loading based on fundamental atomic-scale properties of EM crystals. We report the results of first-principles density-functional calculations of static and thermodynamic properties of PETN, HMX and RDX molecular crystals including properties of different crystalline phases and their equations of states (EOS). The EOS are extended beyond simple isotropic constitutive relationships to include materials response upon uniaxial compressions and high pressures up to 100 GPa. The predictions of the theory are compared with recent experimental results.

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